Three Month Report

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Dr M.Eaton and Dr A.Buchan

1 Introduction

My studies are so far involved with RADIANT (RADIAtion Non-oscillatory Transport), Imperial College's new transport code. I have been implementing the discretisation of energy into the code. This discretisation is now achieved, though the Fission terms will need implementing over the next week, and the convergence needs speeding up, possibly with a Krylov subspace solver. Over the next year, my research will be in the development of discontinuity acceleration methods and space/energy Lanczos solver, and the developement of standard and advanced energy treatments (including step/standard multigroup and space/energy (SUPG) methods.

2 The Boltzmann Neutron Transport Equation

My first task was to research in to the multigroup equations and learn the various discretisation methods used using the main transport code, RADIANT. The main discretisation methods used at streamline upwind Petrov - Galerkin (SUPG) methods which can find solutions to a variaty of problems in radiation and in fluid dynamics. This solver is programmed in FORTRAN, of which I had no prior experience, so whilst in the process of my initial research, I was learning how to program in FORTRAN. My main reference for this report, and much of my work so far is contained in (1) The most important equation in my study is the Boltzmann Neutron Transport Equation, which is defined as follows:

$$\frac{1}{v}\frac{\partial}{\partial t}\psi\left(\vec{r},\hat{\Omega},E,t\right) + \left[\hat{\Omega}\cdot\vec{\nabla}+\sigma\left(\vec{r},E\right)\right]\psi\left(\vec{r},\hat{\Omega},E,t\right) = q\left(\vec{r},\hat{\Omega},E,t\right) \quad (1)$$

over the seven independent variables, space $\vec{r} = (x, y, z)$, angle $\Omega = (\omega, \mu)$ where $cos\chi = \mu$, energy E and time t and v is the speed of the particle. The source q is defined as follows:

$$q\left(\vec{r},\hat{\Omega},E,t\right) = q_{ex}\left(\vec{r},\hat{\Omega},E,t\right) + q_s\left(\vec{r},\hat{\Omega},E,t\right) + q_f\left(\vec{r},\hat{\Omega},E,t\right) \quad (2)$$

The external source, scattering source and fission source respectively.
Using the Bolzmann Neutron Transport Equation, we can follow the discretisation methods used to find an approximate solution.
Firstly, we form the angular discretised form of the multigroup equations,

$$\frac{1}{v}\mathbf{A}_t\frac{\partial\boldsymbol{\psi}\left(\vec{r},t\right)}{\partial t} + \mathbf{A}\cdot\vec{\nabla}\boldsymbol{\psi}\left(\vec{r},t\right) + \boldsymbol{\mathcal{H}}\left(\vec{r},t\right)\boldsymbol{\psi}\left(\vec{r},t\right) - \mathbf{s}\left(\vec{r},t\right) = \mathbf{0} \quad (3)$$

where $\mathbf{A} = \left(\mathbf{A}_x, \mathbf{A}_y, \mathbf{A}_z\right)^T$, $\boldsymbol{\psi}\left(\vec{r},t\right)$ is a vector of the $\mathcal{M}$ angular moments and $\mathcal{H}$ is a $\mathcal{M}\times\mathcal{M}$ matrix which defines the interaction of the radiation with the host media.
We can now use the finite element SUPG formulation of the transport equation, modified by a premultiplication by an SUPG term.
The $\mathcal{M}\times\mathcal{M}$ *angular* matrix $\mathbf{A}_t$ and the three *angular* Jacobian matrices $\mathbf{A}_x$, $\mathbf{A}_y$ and $\mathbf{A}_z$ are defined by:

$$\mathbf{A}_t = \int g(\Omega)g(\Omega)^T d\Omega \qquad \mathbf{A}_k = g(\Omega)\Omega_k g(\Omega)^T d\Omega \qquad k = x, y, z \quad (4)$$

where $g(\Omega)$ is of size $\mathcal{M}$ and contains the basis functions for the angular expansion, and Ω_k are the Cartesian components of the particle direction vector in the $k = x, y, z$

direction, so, $\mathbf{\Omega} = (\Omega_x, \Omega_y, \Omega_z)^T = (\sqrt{1-\mu^2} cos\chi, \sqrt{1-\mu^2} sin\chi, \mu)^T$, where μ is the cosine of the polar angle, and χ is the azimuthal angle in spherical polar coordinates.

$$\left(\mathbf{I} - \mathbf{A} \cdot \vec{\nabla} \mathbf{P}\right) \left(\frac{1}{v} \frac{\partial \mathbf{\Psi}(\vec{r}, t)}{\partial t} + \mathbf{A} \cdot \vec{\nabla} \mathbf{\Psi}(\vec{r}, t) + \mathbf{H}(\vec{r}) \mathbf{\Psi}(\vec{r}, t) - \mathbf{S}(\vec{r}, t)\right) = \mathbf{0} \quad (5)$$

From which we can attain, after a Bubnov - Galerkin discretisation is applied, multiplying by the diagonal matrix $N_i(\vec{r})$ an $\mathcal{M} \times \mathcal{M}$ matrix containing the FE basis functions, integrating over volume and applying Green's theorem, we attain:

$$\begin{aligned} -\int_V \left(\mathbf{A} \cdot \mathbf{N_i}(\vec{r}) \mathbf{\Psi}(\vec{r}, t)\right) dV + \int_V \mathbf{N_i}(\vec{r}) \left(\frac{1}{v} \frac{\partial \mathbf{\Psi}(\vec{r}, t)}{\partial t} + \mathbf{H}(\vec{r}) \mathbf{\Psi}(\vec{r}, t) - \mathbf{S}(\vec{r}, t)\right) dV \\ + \int_V \mathbf{A} \cdot \vec{\nabla} \mathbf{N_i}(\vec{r}) \mathbf{P} \mathcal{R} dV + \int_\Gamma \mathbf{N_i}(\vec{r}) (\mathbf{A} \cdot \mathbf{n}) \mathbf{\Psi}(\vec{r}, t) d\Gamma \\ - \int_\Gamma \mathbf{N_i}(\vec{r}) (\mathbf{A} \cdot \mathbf{n}) \mathbf{P} \mathcal{R} d\Gamma = \mathbf{0} \qquad \forall i \in \{1, 2, ..., \mathcal{N}\} \quad (6) \end{aligned}$$

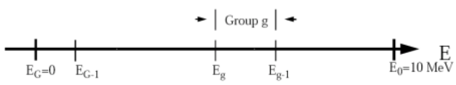
where $\mathbf{n} = (n_x \mathbf{I}, n_y \mathbf{I}, n_z \mathbf{I})^T$ is normal to the boundary Γ of the solution domain V, $\mathbf{I}$ is the Identity matrix of size $\mathcal{M} \times \mathcal{M}$, $\mathbf{P}$ is the SUPG stablisation matrix, and $\mathcal{R}$ is the equation residual defined by

$$\mathcal{R} = \left(\frac{1}{v} \frac{\partial \mathbf{\Psi}(\vec{r}, t)}{\partial t} + \mathbf{A} \cdot \vec{\nabla} \mathbf{\Psi}(\vec{r}, t) + \mathbf{H}(\vec{r}) \mathbf{\Psi}(\vec{r}, t) - \mathbf{S}(\vec{r}, t)\right) \quad (7)$$

and $\mathbf{\Psi}$, $\mathbf{H}$ and $\mathbf{S}$ are the finite element approximations to the functions $\boldsymbol{\psi}$, $\boldsymbol{\mathcal{H}}$ and s respectively.

3 The Multigroup Equation

If we seperate the energy into discrete elements, such as



we can form the multigroup equations which we can use to solve the Boltzmann Neutron Equation after the discretisation of energy:

$$\begin{aligned} \left[\hat{\Omega} \cdot \vec{\nabla} + \sigma_g(\vec{r})\right] \psi_g\left(\vec{r}, \hat{\Omega}\right) = \sum_{g'=1}^{G} \int d\Omega' \sigma_{gg'}\left(\vec{r}, \hat{\Omega}', \cdot \hat{\Omega}\right) \psi_{g'}\left(\vec{r}, \hat{\Omega}'\right) \\ + \frac{1}{k} \chi_g \sum_{g'=1}^{G} v \sigma_{fg'}(\vec{r}) \phi_{g'}(\vec{r}) \quad (8) \end{aligned}$$

for each group $g \in G$ We form the functions ψ_g by integrating over the energy range, so

$$\psi_g\left(\vec{r}, \hat{\Omega}\right) = \int_{E_g}^{E_{g-1}} \psi\left(\vec{r}, \hat{\Omega}, E\right) dE \quad (9)$$

If $f(e)$ is a known function of energy, and the group flux is $\psi_g(\vec{r},\hat{\Omega})$ then we can assume that

$$\psi(\vec{r},\hat{\Omega},E) \approx f(E)\psi_g(\vec{r},\hat{\Omega}) \tag{10}$$

where the energy function is normalised to

$$\int_g f(E)dE = \int_{E_g}^{E_{g-1}} f(E)dE = 1 \tag{11}$$

and expanding out the $\sigma_{gg'}\left(\vec{r},\hat{\Omega}\cdot\hat{\Omega}'\right)$ term into legedre polynomials as below:

$$\sigma_{gg'}\left(\vec{r},\hat{\Omega}\cdot\hat{\Omega}'\right) = \sum_{l=0}^{\infty}(2l+1)\sigma_{lgg'}(\vec{r})P_l(\Omega\cdot\hat{\Omega}') \tag{12}$$

where

$$\sigma_{lgg'}(\vec{r}) = \int_g dE \int_{g'} dE'\sigma_{sl}(\vec{r},E'\rightarrow E)f(E') \tag{13}$$

We can now expand the scattering term so that:

$$\sum_{g'=1}^{G}\int d\Omega'\sigma_{gg'}\left(\vec{r},\hat{\Omega}',\cdot\hat{\Omega}\right)\psi_{g'}\left(\vec{r},\hat{\Omega}'\right) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y^*_{lm}(\hat{\Omega})\sum_{g'=1}^{G}\sigma_{lgg'}(\vec{r})\phi^m_{lg'}(\vec{r}) \tag{14}$$

where $\phi^m_{lg'}$ are the *legendre moments* of the group flux, defined as

$$\phi^m_{lg'}(\vec{r}) = \int d\Omega Y_{lm}(\hat{\Omega})\psi_g(\vec{r},\hat{\Omega}) \tag{15}$$

Once the multigroup equations was programmed, the tolerance level for convergence had to be set. This was achieved through a do loop and a test for convergence for the angular fluxes for each group. To start with, I used a basic tester based on

$$|\psi^i_g - \psi^{i-1}_g| < \epsilon \tag{16}$$

based on the i^{th} iteration for each group, node and moment. However, this might think that a solution has converged when it in fact has not, so to improve upon this method, a Krylov solver is needed to speed up and check for true convergence of the solution. Krylov solvers can speed up the convergence of the solutions and check if the solution is truely converged. The solver we will be using is called IVOR, which the previous loop was used for a preconditioner. Krylov solvers work out the Krylov subspace

$$K_m(A,v) \equiv span(Av, A^2v, A^3v, ..., A^{m-1}v) \tag{17}$$

4 Group Scattering

To begin with, I concentrated on only the group scattering, ignoring the fission term, so the equations I was dealing with were

$$\left[\hat{\Omega}\cdot\vec{\nabla} + \sigma_g(\vec{r})\right]\psi_g\left(\vec{r},\hat{\Omega}\right) = \sum_{g'=1}^{G}\int d\Omega'\sigma_{gg'}\left(\vec{r},\hat{\Omega}',\cdot\hat{\Omega}\right)\psi_{g'}\left(\vec{r},\hat{\Omega}'\right) \tag{18}$$

for each group $g \in G$
Of which the spherical harmonics discrization is:

$$\left[\hat{\Omega} \cdot \vec{\nabla} + \sigma_g\left(\vec{r}\right)\right] \psi_g\left(\vec{r}, \hat{\Omega}\right) = \sum_{g'=1}^{G} \int d\Omega' \sum_{l=0}^{\infty} \left(2l+1\right) \sigma_{lgg'}\left(\vec{r}\right) P_l\left(\hat{\Omega}' \cdot \hat{\Omega}\right) \psi_{g'}\left(\vec{r}, \hat{\Omega}\right) \tag{19}$$

for each group $g \in G$
Now, if we expand out the spherical harmonics, and then simplify, we obtain

$$\left[\hat{\Omega} \cdot \vec{\nabla} + \sigma_g\left(\vec{r}\right)\right] \psi_g\left(\vec{r}, \hat{\Omega}\right) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}^{*}\left(\hat{\Omega}\right) \sum_{g'=1}^{G} \sigma_{lgg'}\left(\vec{r}\right) \phi_{lg'}^{m}\left(\vec{r}\right) \tag{20}$$

where the moments of the group flux are defined as

$$\phi_{lg'}^{m}\left(\vec{r}\right) = \int d\Omega Y_{lm}\left(\hat{\Omega}\right) \psi_g\left(\vec{r}, \hat{\Omega}\right) \tag{21}$$

Next, we have to convert this by the discretisation of energy as a set of linear equations defined upon the streaming operator

$$H_{gg}^{0} \psi_g = \left[\hat{\Omega} \cdot \vec{\nabla} + \sigma_g\left(\vec{r}\right)\right] \psi_g\left(\vec{r}, \hat{\Omega}\right) \tag{22}$$

the group to group operator

$$H_{gg'}^{1} \psi_{g'} = \int d\Omega' \sigma_{gg'}\left(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}'\right) \psi_{g'}\left(\vec{r}, \hat{\Omega}'\right) \tag{23}$$

Then we can define the multigroup transport operator as

$$H_{gg'} = \delta_{gg'} H_{gg}^{0} - H_{gg}^{1} \tag{24}$$

Using the transport operator, we can define a system of equations for the unknowns ψ_g, $g \in G$.

$$\begin{bmatrix} H_{11} & H_{12} & \cdots & H_{1g} & \cdots & H_{1G} \\ H_{21} & H_{22} & & & & \\ \vdots & & \ddots & & & \\ H_{g1} & & & H_{gg} & & \\ & & & & \ddots & \\ H_{G1} & & & & & H_{GG} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_g \\ \vdots \\ \psi_G \end{bmatrix} = \begin{bmatrix} q_1^e \\ q_2^e \\ \vdots \\ q_g^e \\ \vdots \\ q_G^e \end{bmatrix} \tag{25}$$

Or more simply

$$\mathbf{H}\boldsymbol{\psi} = \mathbf{q}^{\mathbf{e}} \tag{26}$$

Now if we discretise in space and angle, we pre-multiply the transport equation but an SUPG term, so that

$$\left(\mathbf{I} - \mathbf{A} \cdot \vec{\nabla} \mathbf{P}\right) \left(\mathbf{A} \cdot \vec{\nabla} \boldsymbol{\Psi}_{\boldsymbol{g}}\left(\vec{r}\right) + \mathbf{H}_{\mathbf{g}}\left(\vec{r}\right) \boldsymbol{\Psi}\left(\vec{r}\right) - \mathbf{S}_{\mathbf{g}}\left(\vec{r}\right)\right) = \mathbf{0} \tag{27}$$

Now, after integrating over space and using Green's theorem, we get

$$
-\int_V (\mathbf{A}\cdot\mathbf{N_i}(\vec{r})\,\boldsymbol{\Psi_g}(\vec{r}))\,dV+\int_V \mathbf{N_i}(\vec{r})\left(\sum_{g'=1}^{G}\mathbf{H_{gg'}}(\vec{r})\,\boldsymbol{\Psi}(\vec{r})-\mathbf{S_{g'}}(\vec{r})\right)dV+
$$

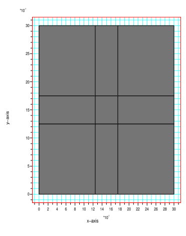
$$
\int_V \mathbf{A}\cdot\vec{\nabla}\mathbf{N_i}(\vec{r})\,\mathbf{P}\mathcal{R}_g dV+\int_\Gamma \mathbf{N_i}(\vec{r})\,(\mathbf{A}\cdot\mathbf{n})\,\boldsymbol{\Psi}_g(\vec{r})\,d\Gamma
$$

$$
-\int_\Gamma \mathbf{N_i}(\vec{r})\,(\mathbf{A}\cdot\mathbf{n})\,\mathbf{P}\mathcal{R}_g d\Gamma=\mathbf{0} \quad (28)
$$

where

$$
\mathcal{R}_g=\left(\mathbf{A}\cdot\vec{\nabla}\boldsymbol{\Psi}_g(\vec{r})+\sum_{g'=1}^{G}(\mathbf{H_{gg'}}(\vec{r})\,\boldsymbol{\Psi}_{g'}(\vec{r})-\mathbf{S}_{g'}(\vec{r})\right) \quad (29)
$$

So, in Radiant, a algorithm for computing the changed terms of the above equation, compared to eq(6) is required. This involved programming a do loop to sum $\int d\Omega'\sigma_{gg'}\left(\vec{r},\hat{\Omega}',\cdot\hat{\Omega}\right)\psi_{g'}$ over the groups and adding this to the right hand side vector. Some of my test results of the multigroup solutions on a simple problem are shown in figures 1 and 2, where the mesh is



and the solutions are: (which are the same solutions as the neutron transport solver, EVENT.)

After this, I started work on extending Radiant to solve with problems up to 6 groups.

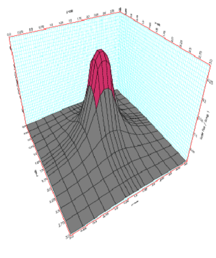


Figure 1: Solution for group 1

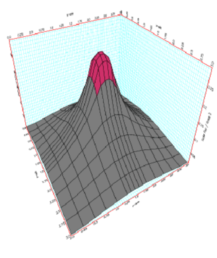
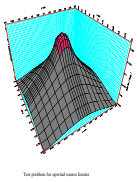
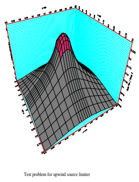


Figure 2: Solution for group 2

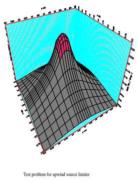
Now, if we use a real life problem, such as the mesh below: We obtain the solutions using RADIANT as



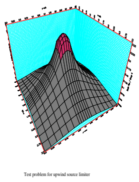
(a) Group 1



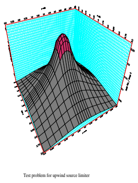
(b) Group 2



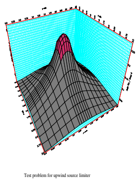
(c) Group 3



(d) Group 4



(e) Group 6



(f) Group 5

Figure 3: The Solutions to the six-group test problem, As you can see from the solutions, the source region is at the peak of the graph showing the scattering of neutrons away from the source, placed in the mesh.

5 Fission

This fission of a multigroup equation is defined as

$$\frac{1}{k}\chi_g \sum_{g'=1}^{G} v\sigma_{fg'}\left(\vec{r}\right)\phi_{g'}\left(\vec{r}\right) \tag{30}$$

Most of the values needed can be taken from WIMS, such as $\chi_g$and $v\sigma_{fg'}$, and the *scalar flux*, $\phi_{g'}$ is defined as

$$\phi\left(\vec{r}\right) = \int \psi_{g'}\left(\vec{r},\hat{\Omega}\right)d\Omega \tag{31}$$

so we need to calculate the *k-eigenvalue*, so defining

$$\mathbf{f}^T = \{v\sigma_{f1}(\vec{r}), v\sigma_{f2}(\vec{r}), \ldots, , v\sigma_{fg}(\vec{r}), \ldots, v\sigma_{fG}(\vec{r})\} \tag{32}$$

and

$$\boldsymbol{\chi}^T = \{\chi_1, \chi_2, \ldots, \chi_g, \ldots, \chi_G\} \tag{33}$$

Then we can rewrite Eq.(30) in vector form:

$$\sum_{g'} v\sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r}) = \mathbf{f}^T(\vec{r})\int \psi(\vec{r},\hat{\Omega})d\Omega \tag{34}$$

and

$$\mathbf{q}_f = \boldsymbol{\chi}\mathbf{f}^T(\vec{r})\int \psi(\vec{r},\hat{\Omega})d\Omega \tag{35}$$

From which we can attain the eigenvalue equation:

$$AF = kF \tag{36}$$

by defining the scalar transport operator as

$$A \equiv \mathbf{f}^T \int \mathbf{H}^{-1}\boldsymbol{\chi}d\Omega \tag{37}$$

and the scalar quantity that defines the spatial distribution of fission neutrons produced in the reactor as

$$F(\vec{r}) = \mathbf{f}(\vec{r})^T \int \psi(\vec{r},\hat{\Omega})d\Omega \tag{38}$$

One of my problems when researching the fission term was how to calculate the operator A. This was due to A not forming a matrix, but being a scalar. Now we have the eigenvalue equation, we need to compute k. The easiest way to do this is by the *power method* algorithm to solve eigenvalue problems, such as in (5) and the power method we are going to use of the problem of the fission eigenvale problem is contained in (2) The power method that we are going to use is as follows:

Algorithm 1 *Power Algorithm for criticality*

1. *Guess core geometry and composition*
2. *Guess inital fission source $S^{(0)}$ and $k^{(0)}$*

3. $M\phi^{(n+1)} = \frac{1}{k^{(n)}} S^{(n)}$
   $S^{(n+1)} = F\phi^{(n+1)}$
   $k^{(n+1)} = \frac{\int d^3 r S^{(n+1)}(\vec{r})}{\frac{1}{k^{(n)}} \int d^3 r S^{(n)}}$

4. *Convergence test*
   $|\frac{k^{(n)} - k^{(n-1)}}{k^{(n)}}| < \epsilon_1$ *and* $|\frac{S^{(n)} - S^{(n-1)}}{S^{(n)}}| < \epsilon_2$

5. *If (3) has not converged then go back to 2*

6. *If (3) has converged then test*
   $k_{eff} \stackrel{?}{=} 1$

7. *if (6) is true then finish*

8. *if (6) is not true go to (1) (Critically search)*

6 Future Research

I will be working to improve the Kylov solver for the multigroup solutions in Radiant over the next month, and in the next few weeks I will be finishing programming the fission term. In the long term, my research will be be based upon the adjoint transport equation looking into problems where we have an object, such as a person, and working backwards to the source of the neutron streams. In the long term, my research will be the paralisation of Radiant, developing discretisation methods for energy building upon the standard step of the mulitgroup equatons. Also in my research plan is the development of goal based metrics for resolving the space/angle mesh. In the second year of my research I will be working on interfacing RADIANT with Rolls-Royce and NEA databank neutron/gamma and covariance data as well GID meshing and MAYAVI and PARAVIEW

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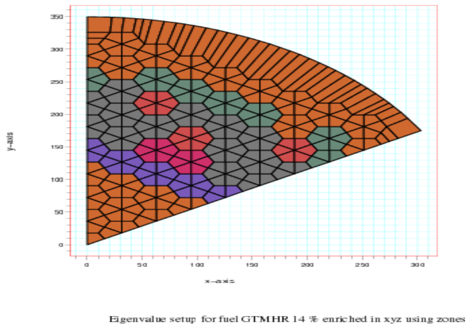
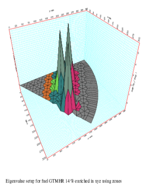
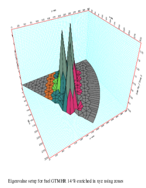


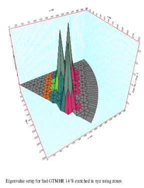
Figure 4: Mesh for real life problem in a reactor



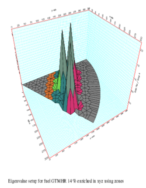
(a) Group 1



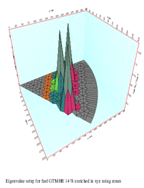
(b) Group 2



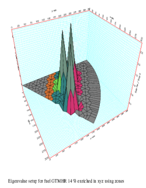
(c) Group 3



(d) Group 4



(e) Group 6



(f) Group 5

Figure 5: The Solutions to the six-group test problem, As you can see from the solutions, the source region is at the peak of the graph showing the scattering of neutrons away from the source, placed in the mesh.